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TITLE A 1-D MODEL FOR HIGHLY SENSITIVE TUBULAR REACTORS

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Abstract. We consider the steady state operation of wall-cooled, fixed-bed tubular reactors. In these reactors the temperature rise ΔT must normally be limited to small fractions of the adiabatic temperature rise ΔT_{ad}, both to avoid runaway and maintain product selectivity. Yet $\Delta T/\Delta T_{ad} << 1$ can only occur if $\eta = t_{dif}/t_{reac} << 1$, where t_{dif} is the timescale on which heat escapes the reactor by "diffusing" to the cooled walls, and t_{reac} is the timescale over which the reaction occurs. So here we use asymptotic methods based on $\eta << 1$ to analyze the 2-d reactor equations, and find the radial concentration and temperature profiles to leading order in η. We then obtain a 1-d model of the reactor by substituting these asymptotically correct profiles into the reactor equations and averaging over r. This model, the α-model, is identical to the standard (Beek and Singer) 1-d model, except that the reactor's overall heat transfer coefficient U is a decreasing function of the temperature rise ΔT. This occurs because as ΔT increases, the reaction becomes increasingly concentrated near $r = 0$, causing a decreased heat transfer efficiency through the reactor's walls. By comparing it with numerical solutions of the original 2-d reactor equations, we find that the α-model simulates the 2-d equations very accurately, even for highly sensitive reactors operated near runaway. We also find that a runaway criterion derived from the α-model predicts the runaway transition of the original 2-d equations accurately, especially for highly sensitive reactors.

1. Introduction. We consider the steady state operation of wall-cooled, fixed-bed tubular reactors. Due to their cost, these reactors are normally used in industry only for highly exothermic reactions. For such reactions, the adiabatic temperature rise ΔT_{ad} is typically several hundred degrees K. Yet reactor runaway occurs when the temperature rise ΔT reaches roughly RT_c^2/E [3-13], which is typically between 15°K and 80°K. So usually ΔT is restricted by

$$1.1 \qquad \Delta T/\Delta T_{ad} \sim RT_c^2/E\Delta T_{ad} << 1$$

and, as we shall see, $\Delta T/\Delta T_{ad} << 1$ can only occur if

$$1.2 \qquad \eta \equiv t_{dif}/t_{reac} << 1,$$

where t_{dif} is the timescale on which heat escapes the reactor by "diffusing" to the cooled walls, and t_{reac} is the timescale on which the reactions occur. So here we use asymptotic methods based on $\eta << 1$ to analyze the reactor.

Specifically, in section 2 we analyze reactors in which a single reaction occurs, and find the radial concentration and temperature profiles to leading order in η. Then, in section 3 we derive a 1-d (z only) model of the reactor by substituting these asymptotically correct profiles into the reactor equations and averaging out r. This model, the α-model, turns out to be identical to the standard (Beek and Singer) 1-d model [1,2], except that the reactor's overall heat transfer coefficient U is not constant, but is a decreasing function of the temperature rise ΔT. This decreased heat transfer efficiency occurs because the reaction, and so the heat generation, become increasingly concentrated near $r = 0$ (away from the reactor walls) as ΔT increases, and is the reason for the known unreliability [1,5,6] of the Beek and Singer model near runaway. In section 3 we compare the α-model with numerical solutions of the original 2-d reactor equations. We

find that the model agrees very well with the 2-d equations, even for highly sensitive reactors operated near runaway. There, we also compare these numerical solutions with the runaway criterion derived from the α-model in [18]. Finally, in section 4 we briefly consider multiple reactions, and extend the α-model to these cases.

2. The 2-d Equations. We choose reactant 1 to be a key reactant and define the conversion X(z,r) by

2.1 $$c^1/\rho \equiv (1-X)c^1_0/\rho_0$$

where ρ is the density of the reacting fluid, and c^j is the molar concentration of species j in the reacting fluid; throughout subscripts 0 refer to the value at the reactor inlet $z = 0$. For the case of a single reaction, all concentrations can be calculated from the conversion [1], so we need only calculate X. In terms of X, the time-independent, pseudo-homogeneous reactor equations are [1,7]

2.2a $$\delta u_0 c^1_0 X_z = \delta c^1_0 D(X_{rr} + \frac{1}{r}X_r) + \tilde{S}(X,T)$$

2.2b $$\delta u_0 \rho_0 c_p T_z = \Lambda(T_{rr} + \frac{1}{r}T_r) + (-\Delta H)\tilde{S}(X,T)$$

inside the reactor $0 < r < r_T$, $0 < z < L$; the boundary conditions are

2.2c $$X_r = 0 \quad , \quad T_r = 0 \qquad \text{at } r = 0$$

2.2d $$X_r = 0 \quad , \quad -\Lambda T_r = h(T - T_c) \qquad \text{at } r = r_T$$

We assume that the reactants enter at the coolant temperature, so

2.2e $\qquad X \equiv 0 \quad , \quad T \equiv T_c \qquad \text{at } z = 0.$

In 2.2, δ is the void fraction of the bed (often denoted by ε), u_0 is the fluid velocity at $z = 0$, and c_p is the fluid's heat capacity. On the right, $\tilde{S}(X,T)$ is the reaction rate, $-\Delta H$ is the heat release of the reaction, D is the effective radial diffusivity of matter, and Λ is the effective radial conductivity of heat. Finally, h is the heat transfer coefficient at the reactor wall.

To nondimensionalize 2.2a - 2.2e effectively, let $\bar{S}$ be a typical value of the reaction rate. To be definite, we choose

2.3a $\qquad \bar{S} \equiv \max_X \tilde{S}(X,T_c).$

Define the dimensionless O(1) reaction rate S by

2.3b $\qquad S(X,T) = \tilde{S}(X,T)/\bar{S}.$

Then in terms of the new variables

2.3c $\qquad r^{new} = r/r_T \quad , \quad z^{new} = z\bar{S}/\delta u_0 c^1{}_0$

the reactor equations become

2.4a $\qquad X_z = \frac{1}{\eta Le}(X_{rr} + \frac{1}{r}X_r) + S(X,T) \quad , \; 0 < r < 1$

2.4b $\qquad \eta T_z = T_{rr} + \frac{1}{r}T_r + QS(X,T) \quad , \; 0 < r < 1$

with

2.4c $\quad X_r = 0 \quad , \quad T_r = 0 \quad$ at $r = 0$

2.4d $\quad X_r = 0 \quad , \quad -T_r = \gamma (T - T_c) \quad$ at $r = 1$

and the initial conditions $X = 0$, $T = T_c$ at $z = 0$. Here,

2.5a $\quad \eta = (\rho_0 c_p r_T^2/\Lambda)(\bar{S}/c^1_0)$

clearly represents the timescale ratio t_{dif}/t_{reac},

2.5b $\quad Le = \Lambda/\delta\rho_0 c_p D$

is the Lewis number, and the constant

2.5c $\quad Q = (-\Delta H)\bar{S} r_T^2/\Lambda$

has the dimension °K and represents the typical temperature rise in the reactor. Finally,

2.5d $\quad \gamma = h r_T/\Lambda$

is the reactor's Biot number. Note that

2.6 $\quad Q/\eta = (-\Delta H)c^1_0/\rho_0 c_p = \Delta T_{ad}$.

From 2.4b we see that ΔT can remain much smaller than ΔT_{ad} only if the heat generation is at

least roughly balanced by the radial diffusion of heat. Since $S(X,T) \sim O(1)$, these terms can only balance when $\Delta T \sim O(Q)$, and thus $\Delta T/\Delta T_{ad} \sim O(\eta)$. So the physical requirement that $\Delta T/\Delta T_{ad} << 1$ implies that $\eta << 1$, as expected.

2.1 Radial profiles. Since $\eta << 1$, 2.4a shows that the radial diffusion of matter is much more rapid than the reaction. So to leading order in η, the conversion is constant in r

2.7 $$X(z,r) = X(z) \qquad \text{for all } r.$$

To obtain the temperature profile, we set $\eta = 0$ in 2.4b and find

2.8a $$(rT_r)_r + rQS(X,T) = 0 \qquad \text{for } 0 < r < 1$$

2.8b $$T_r = 0 \quad \text{at } r = 0, \quad -T_r = \gamma(T - T_c) \quad \text{at } r = 1$$

Now this equation can not be solved explicitly for general reaction rates $S(X,T)$. However, reaction rates generally increase exponentially in T over limited temperature ranges. So consider the expansion

2.9a $$S(X,T) = S(X,\bar{T})e^{A(T - \bar{T})} + \ldots$$

with

2.9b $$A(X,\bar{T}) = \frac{d}{d\bar{T}} \log S(X,\bar{T})$$

around some fixed temperature $\bar{T}$. For example, for Arrhenius kinetics

2.10 $$S(X,T) = a(X)e^{-E/RT} = a(X)e^{-E/R\bar{T}}e^{A(T - \bar{T})} + \ldots$$

with $A = E/R\bar{T}^2$. Solving 2.8 with the reaction rate 2.9, we obtain the radial temperature profile

2.11 $$T(\alpha,r) = T_c + [4\alpha/\gamma - 2\log(1-\alpha+\alpha r^2)]/A$$

where the constant α must satisfy

2.12 $$8\alpha(1-\alpha)e^{-4\alpha/\gamma} = AQS(X,\bar{T})e^{-A(\bar{T}-T_c)}$$

We shall derive our 1-d reactor model by approximating $X(z,r) = X(z)$ and $T(z,r) = T(\alpha,r)$ for some $\alpha(z)$ at each position z in the reactor, and then averaging in r. Note that the Beek and Singer model is derived essentially the same way [1,2], except that the parabolic profiles

2.13 $$T(\beta,r) = T_c + \beta[2/\gamma + 1 - r^2]$$

are used instead of the asymptotically correct profiles 2.11.

3. The 1-d Model. To simplify the eventual 1-d model, define the reaction-averaged temperature $\bar{T}$ by

3.1 $$S(X,\bar{T}) = \langle S(X,T(\alpha,r))\rangle = S(X,\bar{T})\langle e^{A(T-\bar{T})} + \ldots\rangle$$

where $\langle\ \rangle$ denotes the average

3.2 $$\langle f(r)\rangle = \int_0^1 2r\, f(r)\, dr\,.$$

With the radial temperature profile 2.11, 3.1 yields the relation

3.3 $$4\alpha/\gamma - \log(1-\alpha) = A(\bar{T} - T_c)$$

between α and the reaction averaged temperature $\bar{T}$. Substituting $X(z)$ and $T(\alpha,r)$ into the reactor equations 2.4, and averaging now gives

3.4a $$X_z = S(X,\bar{T})$$

3.4b $$\eta\langle T\rangle_z = -8\alpha/A + QS(X,\bar{T}).$$

Now the spatially-averaged temperature $\langle T(\alpha,r)\rangle$ is very nearly the same as the reaction-averaged $\bar{T}$. Since $\eta << 1$, we replace $\langle T\rangle$ by $\bar{T}$ in 3.4b for simplicity. This yields the 1-d model :

3.5a $$X_z = S(X,\bar{T})$$

3.5b $$\eta\bar{T}_z = -8\alpha/A + QS(X,\bar{T}),$$

where

3.5c $$A(X,\bar{T}) = \frac{d}{d\bar{T}} \log S(X,\bar{T})$$

and where the dimensionless heat loss $\alpha(\bar{T})$ is given implicitly by

3.5d $$4\alpha/\gamma - \log(1-\alpha) = A(\bar{T} - T_c).$$

Thus, solving 3.5a - 3.5d requires solving the implicit relation 3.5d to obtain α at each point z; usually one Newton step suffices to update α from the preceding z. Once 3.5a - 3.5d has been solved, then the approximate 2-d solution is

3.5e $\quad X(z,r) = X(z), \qquad T(z,r) = T_c + [4\alpha/\gamma - 2\log(1-\alpha+\alpha r^2)]/A$

Note that for Arrhenius kinetics, $S(X,T) = a(X)e^{-E/RT}$, A is simply $E/R\bar{T}^2$.

3.1 Comparison with the Beek and Singer model. The only real difference between the α-model 3.5a - 3.5e and the Beek and Singer model [1,2] is the term $8\alpha/A$, which represents the heat loss through the reactor walls. To compare the two models, consider the case of Arrhenius kinetics. Then writing the heat loss in terms of an overall heat transfer coefficient U,

3.6 $\quad 8\alpha R\bar{T}^2/E = 2U[\bar{T} - T_c]$

shows that U is a function of the dimensionless temperature rise

3.7a $\quad \phi = E(\bar{T} - T_c)/R\bar{T}^2$

defined implicitly by

3.7b $\quad \dfrac{1}{U} = \dfrac{1}{\gamma} - \dfrac{1}{\phi U}\log(1 - \phi U/4)$

As shown in figure 1, $U(\phi)$ is always a decreasing function of ϕ with

3.8 $\quad U(0) = (\gamma^{-1} + .25)^{-1}$.

Thus, the heat transfer always increases sublinearly with $\bar{T} - T_c$. Now, the Beek and Singer model is exactly 3.5a, 3.5b with the heat transfer term $8\alpha R\bar{T}^2/E$ replaced with the linear term $2U(0)[\bar{T} - T_c]$. So the two models agree when $\phi << 1$ (under "mild" conditions), where the

Beek and Singer model is known to be good [5,6]. Moreover, clearly $U(\phi)$ should decrease because the heat generation becomes increasingly concentrated near the reactor's centerline $r = 0$ as the temperature rise increases, which must lead to a decreased heat transfer efficiency through the reactor walls.

3.2 Comparison with the 2-d equations. The α-model has been tested against the 2-d equations for specific physical reactors elsewhere [17]. So here we consider only the example of a first order Arrhenius reaction $A_1 \rightarrow A_2$, for which

$$3.9 \qquad S(X,T) = (1-X)e^{-E/RT}/e^{-E/RT_c}$$

due to the scaling 2.3a. 2.3b.

The worst errors in the α-model generally occur in predicting the maximum value of $\bar{T}(z)$; this is not surprising since the reactor's heat balance can be very sensitive at its hot spot. Thus, we can rapidly evaluate the α-model's accuracy by testing its predictions of the peak value of $\bar{T}(z)$. To obtain each graph in figure 2 we fixed the value of $Q/\eta = \Delta T_{ad}$ and varied η. For each η we solved the original 2-d equations, the α-model, and the Beek and Singer model; we then found and graphed the maximum value of $\bar{T}(z)$ from each calculation. Additionally, figure 3 shows the full $X(z)$ and $\bar{T}(z)$ curves for an extreme case. In figure 2, we see that significant errors in the α-model occur only for the least exothermic reaction considered (figure 2d), and then they occur only when $\bar{T}(z) - T_c$ exceeds 50°K. Note that when $\bar{T}(z) - T_c$ is 50°K, the value of $T(z,r) - T_c$ is already a severe 80°K at $r = 0$.

We have tested the α-model on many other examples [16,17]. Our general experience is that the α-model simulates the original 2-d equations very accurately for highly sensitive reactors which have sharp runaway transitions as in figures 2a and 2b; for less sensitive reactors which have "soft" runaway transitions as in figure 2d, significant errors can occur, but only when the

temperature rise ΔT is very severe. For example, for a single Arrhenius reaction the accuracy improves as $E\Delta T_{ad}/RT_c^2$ increases, as RT_c/E decreases, and as the reaction order decreases.

3.3. Runaway. Very sophisticated methods have been used to analyze the Beek and Singer model to develop runaway criteria [4,13]. However, these criteria are necessarily limited by the accuracy of the Beek and Singer model near runaway (see figure 2). In [18] we obtained a new criterion by using asymptotic methods based on $\eta << 1$ to analyze the more accurate α-model. For the special case of Arrhenius kinetics

3.10 $$S(X,T) = a(X)e^{-E/RT}$$

with the maximum of $a(X)$ occurring at $X = 0$ (positive reaction order), this criterion predicts runaway when

3.11a $$\eta a(0)e^{-E/RT_c} > \frac{1+\varepsilon}{P} f(\gamma)\left\{1 + 2.946(1+\varepsilon)\left|\frac{g(\gamma)a'(0)}{Pa(0)}\right|^{2/3}\right\}$$

Here ε and P depend only on the chemical reaction

3.11b $$\varepsilon = RT_c/E, \qquad P = E\Delta T_{ad}/RT_c^2$$

and f and g depend only on the Biot number γ

3.11c $$f = 8\beta(1-\beta)e^{-4\beta/\gamma}, \qquad g = (1-\beta)/\sqrt{1-2\beta+2\beta^2}$$

through

3.11d $$\beta(\gamma) = \frac{1}{4}(\gamma+2-\sqrt{\gamma^2+4})$$

Note that for equi-molar reactions, $|a'(0)/a(0)|$ is just the reaction order.

This criterion can be evaluated readily from peak temperature curves like figures 2a - 2d, which show the reactor's runaway transition quite clearly. In figure 2, the points where equality occurs in 3.11a have been marked with solid points. For the two most exothermic reactions in figure 2, the runaway transition is quite sharp and the runaway criterion is quite accurate. For the two least exothermic reactions, the transition is not sharp, so the point where runaway first occurs cannot be defined precisely. In view of this theoretical indeterminacy, the points obtained from 3.11 still seem quite reasonable.

4. Multiple Reactions. Suppose that there are n reactions occurring in the reactor. Then all concentrations can be expressed in terms of n variables $\underline{X} = (X^1, X^2, ..., X^n)$, each measuring the extent of one of the reactions. Similar to 2.4a - 2.4d, the dimensionless reactor equations can be written as

4.1a $$X^j{}_z = \frac{1}{\eta Le}(X^j{}_{rr} + \frac{1}{r}X^j{}_r) + S^j(\underline{X},T) \qquad j = 1, ..., n$$

4.1b $$\eta T_z = T_{rr} + \frac{1}{r}T_r + \sum_j Q^j S^j(\underline{X},T)$$

for $0 < r < 1$, with the same boundary conditions 2.4c, 2.4d as before. To obtain the α-model we approximate the temperature dependence of the total heat release $\sum Q^j S^j(\underline{X},T)$ as exponential; then 2.11 gives the asymptotically correct profiles $T(\alpha,r)$; and substituting these profiles into the reactor equations and averaging over r yields :

4.2a $$X^j{}_z = S^j(\underline{X},\overline{T}) \qquad j = 1, ..., n$$

4.2b $$\eta \overline{T}_z = -8\alpha/A + \sum_j Q^j S^j(\underline{X},\overline{T})$$

where

4 2c $$A(\underline{X},\bar{T}) = \frac{\partial}{\partial \bar{T}} \log [\Sigma\, Q^j S^j(\underline{X},\bar{T})]$$

and where α is determined by

4.2d $$4\alpha/\gamma - \log(1-\alpha) = A(\bar{T} - T_c) .$$

Once 4.2a - 4.2d have been solved, then the approximate 2-d solution is

4.2e $$X^j(z,r) = X^j(z), \qquad T(z,r) = T_c + [4\alpha/\gamma - 2\log(1-\alpha+\alpha r^2)]/A .$$

This model has been tested with experimentally derived reaction schemes in [17,19]. So here we consider the example of two first-order Arrhenius reactions $A_1 \rightarrow A_2$, $A_1 \rightarrow A_3$, with the second reaction having twice the activation energy of the first, and with both reactions releasing equal amounts of heat, so $Q^1 = Q^2 = Q$. We also choose the reaction rates

4.3a $$S^1(\underline{X},T) = .80(1-X^1-X^2)e^{-E/RT_\theta + E/RT_c}$$

4.3b $$S^2(\underline{X},T) = .20(1-X^1-X^2)e^{-E/RT_\theta + E/RT_c}$$

so that the second is 25% of the first at $T = T_c$. As in figure 2, in figure 4 we graph the peak value of $\bar{T}(z)$ as a function of η with $Q/\eta = \Delta T_{ad}$ held fixed. The accuracy of the α-model for this case should not be surprising since the reactor is clearly extremely sensitive.

5. Conclusions. The α-model and runaway criterion have been tested on many other examples in [16-19]. In particular, in [18] we observe that the maximum feasible reaction rates occur when the reactor reaches runaway. So there we use the runaway criterion to determine the theoretical limits

on the reactor's performance.

We have found the α-model, the runaway criterion, and the theoretical limits to be useful in rapidly screening potential reactor designs and operating conditions to assess relative reactor performances and sensitivities. Once the final design and operating conditions have been settled, we have then solved the 2-d equations to verify the predictions of the model.

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Figure captions.

Figure 1. The dimensionless heat transfer coefficient $U(\phi)$ and heat loss $\alpha(\phi)$.

Figure 2. The peak value of $\bar{T}(z)$ in the reactor as a function of η. Shown are the predictions of the α-model (α), the Beek and Singer model (s), and the exact values from the 2-d equations (e). There are no significant differences between the predictions of the α-model and the 2-d equations in figures 2a-2c. The values of $P = EQ/\eta RT_c^2 = E\Delta T_{ad}/RT_c^2$ are 40, 20, 12, and 8 in figures 2a-2d, respectively. The other parameter values are $RT_c/E = .10$, $\gamma = 4.8$, $T_c = 500°K$, and $Le = 1.25$.

Figure 3. The axial profiles $\bar{T}(z)$ and $X(z)$ from the α-model (α), the Beek and Singer model(s), and the exact values (e). The values $E\Delta T_{ad}/RT_c^2 = 20$ and $\eta = .12$ have been chosen so that the reactor is very near runaway (see figure 2b), causing a very pronounced hot spot. The other parameter values are as in figure 2.

Figure 4. The peak value of $\bar{T}(z)$ in the reactor as a function of η for two simultaneous first-order reactions (see equation 4.3). Shown are the predictions of the α-model (α), the Beek and Singer model (s), and the exact values (e). There is no discernable difference between the exact values and the predictions of the α-model. The parameters are $E\Delta T_{ad}/RT_c^2 = 20$, $RT_c/E = .10$, $\gamma = 4.8$, $T_c = 500°K$, and $Le = 1.25$.

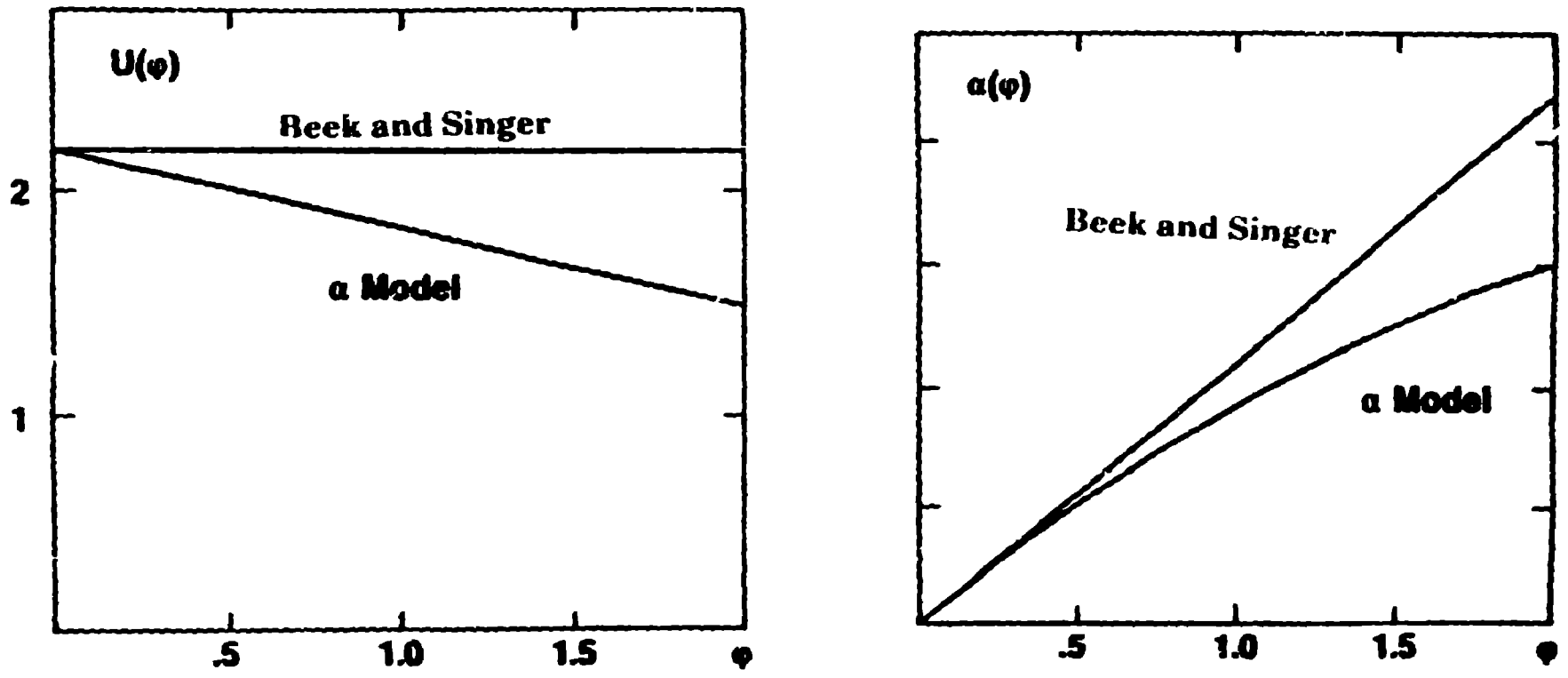
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Figure 1

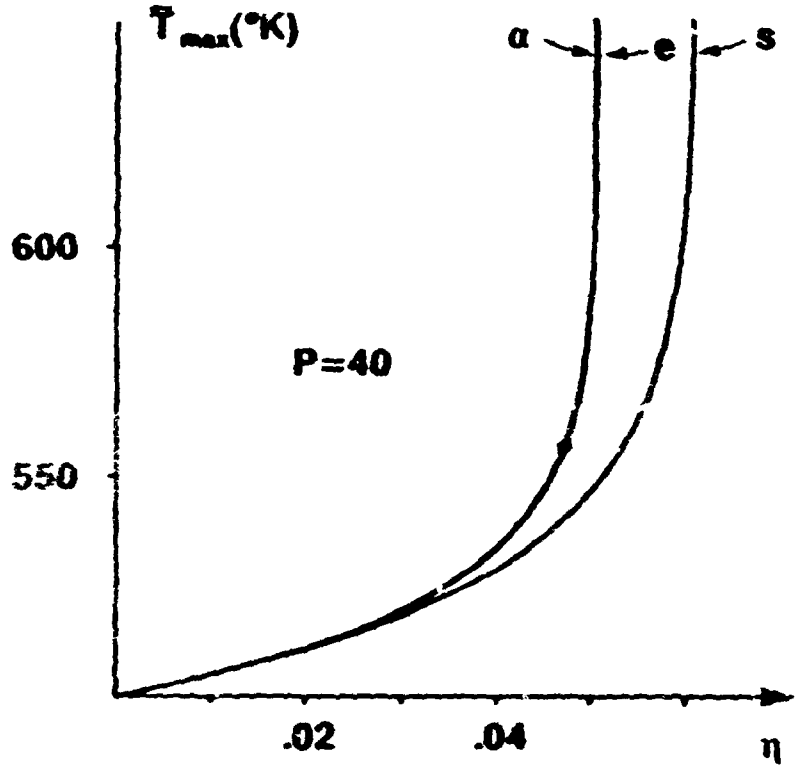


Figure 2a

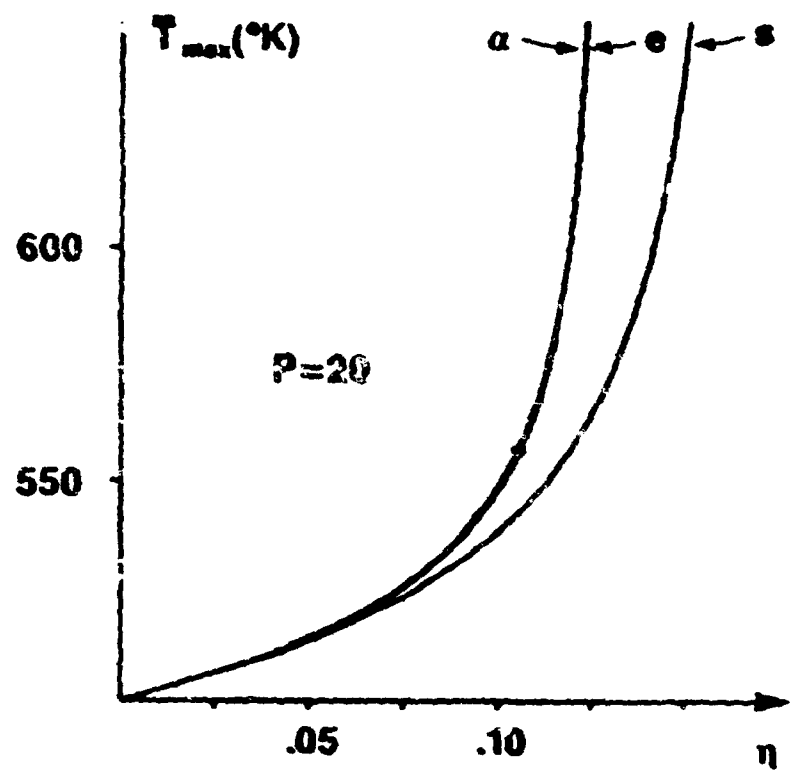


Figure 2b

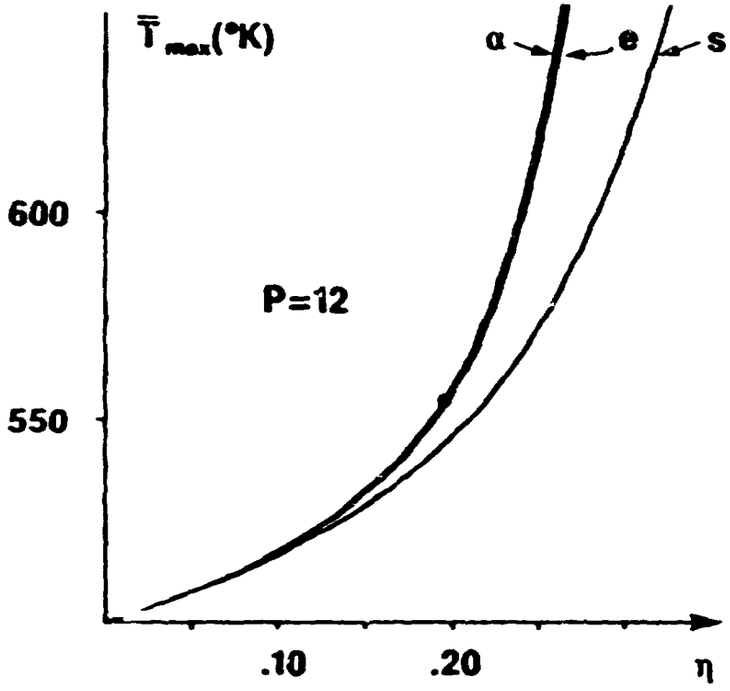


Figure 2c

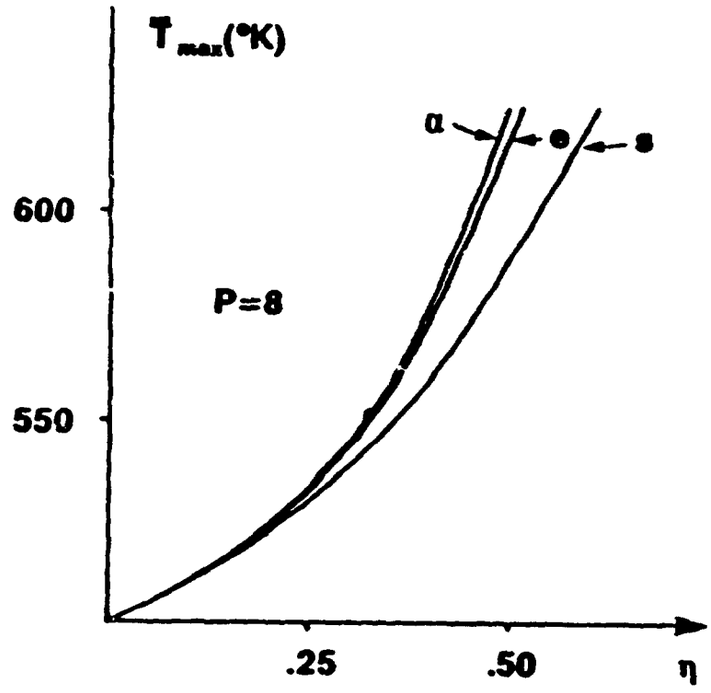
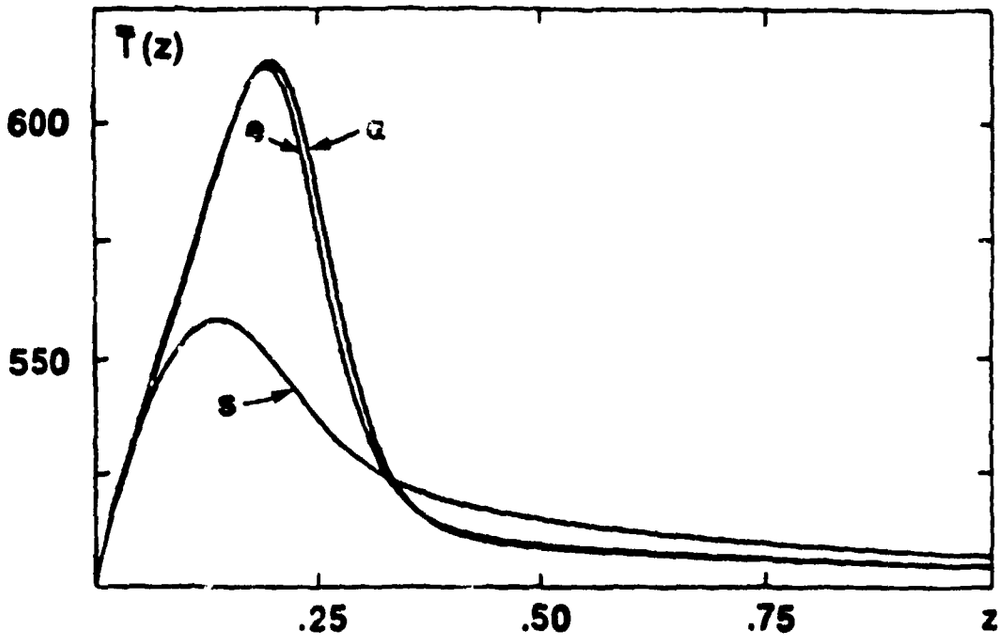


Figure 2d



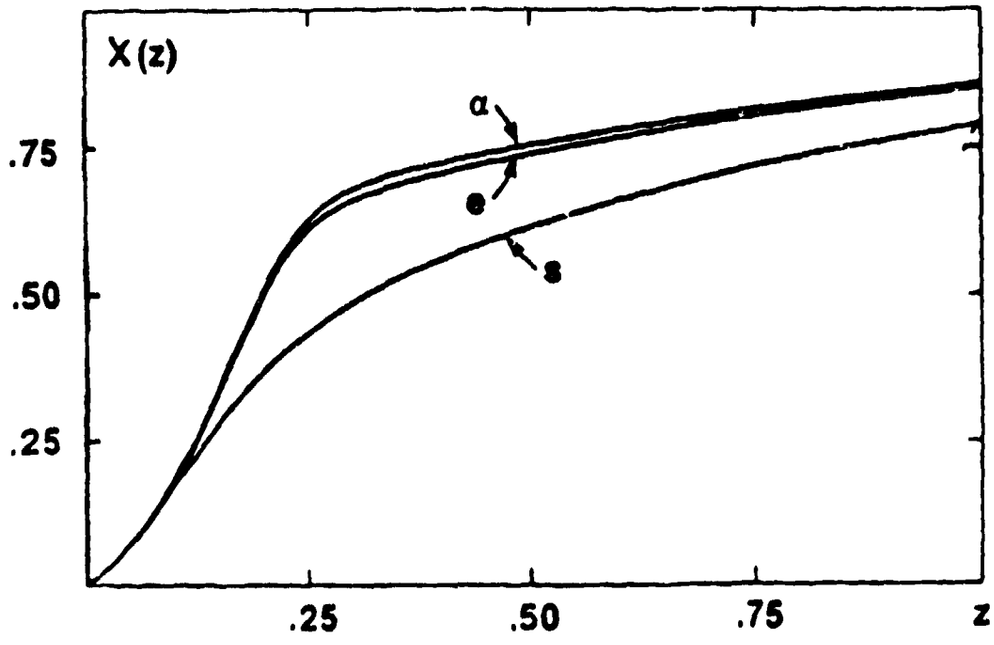


Figure 3

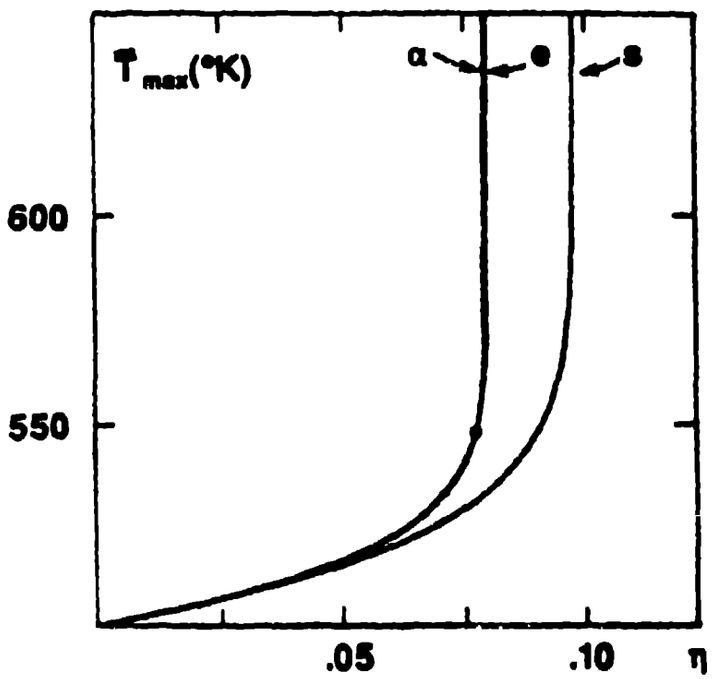


Figure 4